

1,4-Diazabicyclo[2.2.2]octane
280-57-9 | DTXSID0022016

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 44.7 days

Global applicability domain: Outside

Local applicability domain index: 1.58e-01

Confidence level: 7.14e-01

Nearest Neighbors from the Training Set

Image not found

2,2,3-Trimethylbutane

Measured: 61.9

Predicted: 10.7

Image not found

2,3,4-Trimethylpentane

Measured: 511

Predicted: 13.9

Image not found

Adamantane

Measured: 8090000

Predicted: 968

Image not found

Cyclohexane

Measured: 8170

Predicted: 34.7

Image not found

2,2,4-Trimethylpentane

Measured: 4890

Predicted: 30.5